mit

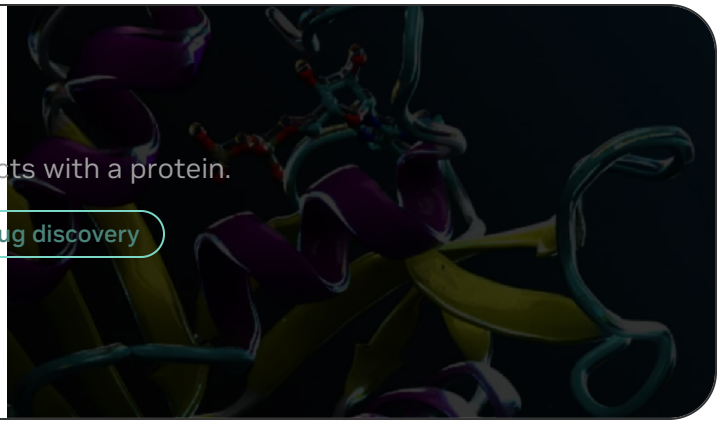
diffdock

Run Anywhere

Predicts the 3D structure of how a molecule interacts with a protein.

bionemo chemistry docking nim drug discovery

Get API Key



AI models generate responses and outputs based on complex algorithms and machine learning techniques, and those responses or outputs may be inaccurate, harmful, biased or indecent. By testing this model, you assume the risk of any harm caused by any response or output of the model. Please do not upload any confidential information or personal data unless expressly permitted. Your use is logged for security purposes.

Input

Try Python Shell

View Examples

Molecule * ⓘ

Ensitrelvir_analog_3d.sdf

File Types: .sdf | .mol2 Upload New File

Target Protein * ⓘ

mpro_chain_OpenFold_proc...

File Types: .pdb Upload New File

Generated Poses ⓘ

Output

Preview Ascii

{"title":"{\"type\":\"urn:inference-service:problem-details:internal-server-error\",\"title\":\"Internal Server Error\",\"status\":500,\"detail\":\"Inference error\"}"}

Diffusion Steps ⓘ

24

1 11 21 31 40

18

1 3 5 7 9 11 13 15 17 19 20

Diffusion Time Divisions ⓘ

20

3 5 7 9 11 13 15 17 19 20

Reset Run